Professor Sebastian Kozuch

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Friday, July 14th at 11:00am 36-144

On the kinetics of catalysis

Abstract: With the development of computational tools the calculation of reaction pathways for catalytic systems has become a routine job. But still, a missing link between the calculated reaction profile and the kinetics of a catalytic cycle makes it challenging to resolve the basic question: What makes for a good catalytic cycle? The Energy Span Model is a kinetic methodology that permits the calculation of the TOF (turn-over frequency) and TON (turn-over number) of catalytic networks from their energy representation. In other words, it provides a mathematical tool that enables:

- I) To choose the right mechanism among all the alternative possibilities.
- II) To understand the fundamental factors that shape the kinetics of a catalytic network.
- III) To suggest improvements for a catalyst.

Biography: Sebastian Kozuch was born in Argentina, and studied his first chemical degree at the University of Buenos Aires. Then he moved to Jerusalem to do an MSc and PhD with Sason Shaik, and then a first postdoc at the Weizmann Institute with Jan Martin. After that he went to the University of North Texas for a second postdoc with Wes Borden. And finally he moved to Ben-Gurion University of the Negev almost three years ago, where he is an assistant professor.

Hosted by Professor Heather J. Kulik, Chemical Engineering Department See the doodle poll: <u>http://doodle.com/poll/fit6g2nui27pkddk</u> if you would like to meet with Prof. Kozuch during his visit.